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The effect of antiferromagnetic spin fluctuations on the uniform spin susceptibility in high-T_c superconductors

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Abstract. In this paper we developed a theory for the effect of antiferromagnetic spin fluctuations on the uniform spin susceptibility. Our theoretical analysis suggests strongly that the effect of the antiferromagnetic spin fluctuations on the uniform spin susceptibility is the origin of the temperature dependence of the uniform spin susceptibility in high-T_c superconductors.

1. Introduction

It is well known that the most striking features of high-T_c oxides are their anomalous physical properties above their transition temperatures T_c. For example the electrical resistivity is linear in temperature in a wide range of temperatures above T_c, the infrared conductivity deviates from the Drude form, showing a relaxation rate proportional to the frequency, and the nuclear spin–lattice relaxation rate shows an anomalous temperature dependence different from that in normal metals, etc [1, 2].

The above-mentioned anomalous physical properties have been explained in terms of antiferromagnetic spin fluctuations in two-dimensional metals [3–9]. Their uniform spin susceptibility $\chi(T)$, which displays a considerable temperature dependence, has been explained in terms of a pseudo-spin gap [10]. However, the role of the pseudo-spin gap in the antiferromagnetism of the high-T_c Cu oxides has not yet been elucidated. We expect naturally that the antiferromagnetic spin fluctuations affect the uniform spin susceptibility and lead to the temperature dependence.

The rest of the paper is organized as follows. In section 2 we develop a theory of the effect of the antiferromagnetic spin fluctuations on the uniform spin susceptibility, on the basis of the self-consistent renormalization (SCR) theory of spin fluctuations [11, 12] which goes one step beyond the Hartree–Fock–RPA theory and treats the renormalized spin fluctuations and the renormalized thermal equilibrium state in a self-consistent fashion. In section 3 we discuss our results and compare them with experimental data. The paper concludes with a summary in section 4.

2. Theory

Following [13, 14] except for the external magnetic field, the Hamiltonian is given by

$$H = \sum_k \hat{C}_k^+(\varepsilon_k - \tau_3 h_0)\hat{C}_k - \tfrac{1}{2}I^2 \sum_k \chi(k) S(k) \cdot S(-k) \qquad (2.1)$$

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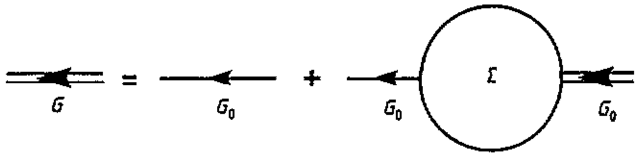

Figure 1. The graphical equation relating G to G_0 and the self-energy Σ: single line plus arrow, unperturbed Green function G_0; double line plus arrow, the one-particle Green function G; Σ in circle, the self-energy Σ.

where $k = (\boldsymbol{k}, \omega_k)$ is the four-vector, $S(k)$ is the electron-spin operator, I is the coupling constant, $\chi(k)$ is the spin susceptibility, ε_k is the kinetic energy measured from the Fermi level, τ_i ($i = 1, 2, 3$) is the Pauli matrix, h_0 is the external magnetic field, $\hat{C}_k^+(c_{k\uparrow}^+, c_{k\downarrow}^+)$ and $c_{k\sigma}^+$ is the electron creation operator with spin σ. We treat h_0 and the interaction as a perturbation, as illustrated in figures 1 and 2. Using the unperturbed Green function $G_0(k, \mathrm{i}\omega_k) = (\mathrm{i}\omega_k - \varepsilon_k)^{-1}$ we find that the one-particle Green function for this system may be written $G^{-1} = G_0^{-1} - \Sigma$, where Σ is the self-energy, as shown in figure 2. From figure 2 we have

$$\Sigma(p) = \Sigma_0 + \Sigma_1(p) + \Sigma_2^a(p) + \Sigma_2^b(p) \tag{2.2}$$

$$\Sigma_0 = -\tau_3 h_0 \tag{2.2a}$$

$$\Sigma_1(p) = \frac{I^2}{\beta}\sum_{ki}\chi(p-k)\tau_i G_0(k)\tau_i \tag{2.3a}$$

$$\Sigma_2^a(p) = -\frac{I^2}{\beta}\sum_{ki}\chi(p-k)\tau_i G_0(q+k)h_0\tau_3 G_0(k)\tau_i \tag{2.4a}$$

$$\Sigma_2^b(q) = -\frac{I^2}{\beta}\chi(q)\sum_{ki}\tau_i G_0(k)h_0\tau_3 G_0(k+q)\tau_3. \tag{2.5a}$$

Use

$$\chi(p-k) = -\int_{-\infty}^{+\infty}\frac{\mathrm{d}z}{\pi}\frac{\mathrm{Im}[\chi(\boldsymbol{p}-\boldsymbol{k}, z)]}{\mathrm{i}(\omega_p - \omega_k) - z}$$

and perform the summation over ω_k. Then equations (2.3a), (2.4a) and (2.5a) reduce to

$$\Sigma_1(\boldsymbol{p}, \mathrm{i}\omega_p) = 3I^2\sum_{\boldsymbol{k}}\int_{-\infty}^{+\infty}\frac{\mathrm{d}z}{\pi}\mathrm{Im}[\chi(\boldsymbol{p}-\boldsymbol{k}, z)]\frac{b(z) + f(\varepsilon_k)}{\mathrm{i}\omega_p + z - \varepsilon_k} \tag{2.3b}$$

$$\Sigma_2^a(\boldsymbol{p}, \mathrm{i}\omega_p) = h_0\tau_3 I^2\sum_{\boldsymbol{k}}\int_{-\infty}^{+\infty}\frac{\mathrm{d}z}{\pi}\mathrm{Im}[\chi(\boldsymbol{p}-\boldsymbol{k}, z)]\frac{1}{\varepsilon_k - \varepsilon_{k+q} + \mathrm{i}\omega_q} \times\left(\frac{b(z) + f(\varepsilon_k)}{\mathrm{i}\omega_p + z - \varepsilon_k} - \frac{b(z) + f(\varepsilon_{k+q})}{\mathrm{i}(\omega_p + \omega_q) + z - \varepsilon_{k+q}}\right) \tag{2.4b}$$

$$\Sigma_2^b(q, \mathrm{i}\omega_q) = h_0\tau_3 I^2\chi(q)\sum_{k}\frac{b(z) + f(\varepsilon_{k+q})}{\mathrm{i}\omega_q + \varepsilon_k - \varepsilon_{k+q}} \tag{2.5b}$$

where b and f are the Bose and Fermi distribution functions, respectively.

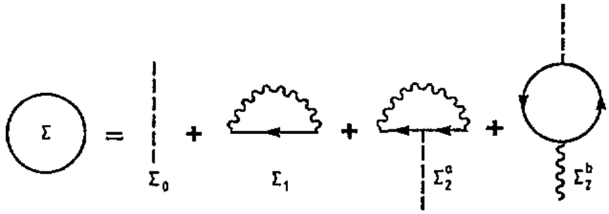

Figure 2. The most important contribution to the self-energy $\Sigma(p)$ from the antiferromagnetic spin fluctuation and the external magnetic field: wavy line, the spin fluctuation propagator; ——, the electron propagator; - - - -, the external magnetic field.

Make a further approximation for the self-energy, i.e. first take the limit $q \to \mathbf{0}$ and then the limit $\omega_q \to 0$. We get

$$\Sigma_2^a(p, \mathrm{i}\omega_p) \simeq h_0 \tau_3 I^2 \sum_k \int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{\pi} \operatorname{Im}[\chi(p-k, z)] \frac{b(z) + f(\varepsilon_k)}{(\mathrm{i}\omega_p + z - \varepsilon_k)^2} \tag{2.4c}$$

$$\Sigma_2^b(0, 0) \simeq 0. \tag{2.5c}$$

We are only interested in $\operatorname{Re}[\Sigma(p, \omega)]$. By analytical continuation ($\mathrm{i}\omega_p \to \omega + \mathrm{i}\delta$) we obtain the real part of the self-energy:

$$\operatorname{Re}[\Sigma(p, \omega)] = \operatorname{Re}[\Sigma_1(p, \omega)] - h_0 \tau_3 \frac{1}{3} \frac{\partial}{\partial \omega} \operatorname{Re}[\Sigma_1(p, \omega)] - \tau_3 h_0 \tag{2.6}$$

with

$$\operatorname{Re}[\Sigma_1(p, \omega)] = 3I^2 \sum_k \int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{\pi} \operatorname{Im}\left(\chi(p-k, z) \frac{b(z) + f(\varepsilon_k)}{\omega + z - \varepsilon_k}\right). \tag{2.6a}$$

According to the SCR theory for weak itinerant antiferromagnets, the dynamical susceptibility around the staggered component is given by [11, 12]

$$\chi_{Q+q}(\omega, T) = \frac{\chi_{Q+q}(T)}{1 + \mathrm{i}\omega / \Gamma_{Q+q}} \tag{2.7}$$

with

$$\chi_{Q+q}(T) = \chi_Q(T)/(1 + q^2/k_s^2)$$
$$\Gamma_{Q+q} = \Gamma_s(k_s^2 + q^2)$$
$$k_s^2 = \chi_Q^0 / A\chi_Q(T)$$

where Q is the wavevector specifying the antiferromagnetic order, χ_Q^0 is the susceptibility in the absence of the electron–electron interaction I, k_s is the inverse antiferromagnetic correlation length, and the parameters Γ_s and A specify the frequency spread and the spatial correlation of the spin fluctuations, respectively. The staggered susceptibility $\chi_Q(T)$ is obtained by solving the following equations which take account of the coupling between the spin fluctuation modes around $q = Q$ (equations (3) and (4) in [12]):

$$\frac{1}{\chi_Q(T)} = \frac{1}{\chi_Q^{\mathrm{HF}}} + \tfrac{5}{3} F_s S_L^2(T) \tag{2.8}$$

with

$$S_L^2(T) = \frac{3}{2\pi} \int \mathrm{d}\omega \coth\left(\frac{\omega}{2T}\right) N^{-2} \sum_q \mathrm{Im}[\chi_{Q+q}(\omega, T)]$$

where χ_Q^{HF} is the Hartree–Fock result: $\chi_Q^{\mathrm{HF}} = \chi_Q^0/(1-\alpha_Q)$. $(1-\alpha_Q)^{-1}$ is the exchange enhancement factor. The second term in equation (2.8) represents the mode–mode coupling. Since equations (2.7) and (2.8) for $\chi_{Q+q}(\omega, T)$ contain $\chi_Q(T)$, equations (2.7) and (2.8) must be solved consistently for $\chi_Q(T)$. Following [13, 14], when $\omega \ll T$, from equations (2.6*a*) and (2.7) we have

$$\mathrm{Re}[\Sigma_1(\boldsymbol{p}_{\mathrm{F}}, \omega)] = -3\omega I^2 \int \frac{\mathrm{d}\theta_k}{2\pi} N_0(\theta_k) \frac{\chi_Q(T)\Gamma_s k_s^2}{\Gamma_{\boldsymbol{p}-\boldsymbol{k}}} \tag{2.9}$$

where the wavevectors $\boldsymbol{k}$ and $\boldsymbol{p}$ are restricted to lie on the Fermi surface, which is assumed to be topologically simple, θ_k is an angle parametrizing the Fermi surface, and $N_0(\theta_k)$ is the density of states at the angle θ_k. Define $\Gamma_{\min}(\theta_{k\,\min}, \theta_p)$ as the minimum as $\boldsymbol{k}$ ranges over the Fermi surface of $\Gamma_s[k_s^2 + |\boldsymbol{p} - \boldsymbol{k} - \boldsymbol{Q}|^2]$. The dependence on the angle away from the minimum value is quadratic, i.e.

$$\Gamma(\theta_k, \theta_p) = \Gamma_{\min}(\theta_{k\,\min}, \theta_p) + \tfrac{1}{2}\Gamma_s |\boldsymbol{k}_{\mathrm{F}}|^2 (\theta_k - \theta_{k\,\min})^2. \tag{2.10}$$

Substituting this into (2.9) and integrating give

$$\mathrm{Re}[\Sigma_1(\boldsymbol{p}_{\mathrm{F}}, \omega)] = -\omega 3 I^2 \frac{N_0 \chi_Q(T)\Gamma_s k_s^2}{(2)^{1/2}\pi(\Gamma_{\min}\Gamma_s|\boldsymbol{k}_{\mathrm{F}}|^2)^{1/2}} \tan^{-1}\left(\frac{\Gamma_s|\boldsymbol{k}_{\mathrm{F}}|^2}{2\Gamma_{\min}}\right)^{1/2} \tag{2.11}$$

$\mathrm{Re}[\Sigma_1(\boldsymbol{p}_{\mathrm{F}}, \omega)]$ is a function of the angle parametrizing the Fermi surface. As quite often its average value is given for a metal [15], by averaging $\mathrm{Re}[\Sigma_1(\boldsymbol{p}_{\mathrm{F}}, \omega)]$ over the Fermi surface we obtain

$$\mathrm{Re}\left[\overline{\Sigma_1(\boldsymbol{p}_{\mathrm{F}}, \omega)}\right] = -3\lambda\omega \tag{2.12}$$

with

$$\lambda = B[\chi_Q(T)]^{1/2} \tan^{-1}[C\chi_Q(T)]^{1/2} \qquad B \simeq I^2 N_0 \frac{1}{\sqrt{2}\pi k_{\mathrm{F}}} \left(\frac{\chi_Q^0}{A}\right)^{1/2} \qquad C \sim \frac{|\boldsymbol{k}_{\mathrm{F}}|^2}{2} \frac{A}{\chi_Q^0}.$$

Inserting equation (2.12) into (2.6) we get

$$\mathrm{Re}\left[\overline{\Sigma(\boldsymbol{p}_{\mathrm{F}}, \omega)}\right] = -h_0\tau_3 - 3\lambda\omega + h_0\tau_3\lambda. \tag{2.13}$$

Near the Fermi surface the renormalized Green function under the external field h_0 is

$$G(k,\omega) = \frac{1}{z}\frac{1}{\omega - \tilde{E}_k + \mathrm{i}\delta}$$

with

$$z = \frac{1}{3\lambda+1} \qquad \tilde{E}_k = \tilde{\varepsilon}_k = \tau_3\frac{1-\lambda}{3\lambda+1}h_0 \qquad \tilde{\varepsilon}_k = \frac{\varepsilon_k}{3\lambda+1}.$$

Following [16], to find the magnetization M we need only to compute the difference between the numbers of up- and down-spin quasi-particles:

$$M = \int_{-\infty}^{+\infty}\left[D(\tilde{\varepsilon}_k) f\left(\tilde{\varepsilon}_k - \frac{1-\lambda}{3\lambda+1}h_0\right) - D(\tilde{\varepsilon}_k) f\left(\tilde{\varepsilon}_k + \frac{1-\lambda}{3\lambda+1}h_0\right)\right]\mathrm{d}\tilde{\varepsilon}_k.$$

We expand the Fermi function about $h_0 = 0$ to yield

$$M = 2\frac{1-\lambda}{3\lambda+1}h_0\int_0^{\infty}\left(-\frac{\partial f}{\partial\tilde{\varepsilon}_k}\right)D(\tilde{\varepsilon}_k)\,\mathrm{d}\tilde{\varepsilon}_k.$$

This leads to the uniform spin susceptibility

$$\chi(T) = \lim_{h_0\to 0}\left(\frac{M}{h_0}\right) = \chi^0 - \lambda\chi^0 \tag{2.14}$$

where

$$\chi^0 = \frac{2}{3\lambda+1}\int_0^{\infty}\left(-\frac{\partial f}{\partial\tilde{\varepsilon}_k}\right)D(\tilde{\varepsilon}_k)\,\mathrm{d}\tilde{\varepsilon}_k$$

is the uniform spin susceptibility for considering only Stoner exchange enhancement, which is approximately temperature independent (see figure 4(*a*) in [4]). Inserting equation (2.12) into equation (2.14) we get

$$\chi(T) = \chi^0 - B'[\chi_Q(T)]^{1/2}\tan^{-1}[C\chi_Q(T)]^{1/2} \tag{2.15}$$

with $B' = \chi^0 B$. Equation (2.15) shows that the uniform spin susceptibility is affected by the antiferromagnetic spin fluctuations. In the following section, we discuss our results and compare them with experiment.

3. Comparison with experiment

From the result of the previous section the uniform spin susceptibility can be expressed by the following formula:

$$\chi(T) = \chi^0 - B'[\chi_Q(T)]^{1/2}\tan^{-1}[C\chi_Q(T)]^{1/2} \tag{3.1}$$

where χ^0 represents the uniform spin susceptibility considering only the Stoner exchange enhancement. The second term represents the effect of the antiferromagnetic spin fluctuations on the uniform spin susceptibility. For simplicity we use the experimental values [17, 18] of the staggered susceptibility for $\chi_Q(T)$.

Fro $YBa_2Cu_3O_{6.63}$ ($T_c = 60$ K) the least-squares fit of the theoretical equation (3.1) to the experiment [18, 19] yields the following result:

$$\chi(T) = 3 - \frac{18.33}{(T+30)^{1/2}} \tan^{-1}\left(\frac{35}{(T+30)^{1/2}}\right). \tag{3.2}$$

In figure 3 a plot of $\chi(T)$ versus T for $YBa_2Cu_3O_{6.63}$ is shown. The solid curve shows the values from equation (3.2). The following values are used for the parameters in the fit: $\chi^0 = 3$ eV^{-1}, $B' = 0.31$ eV$^{1/2}$ and $C = 0.34$ eV. On the other hand by using $I^2 N_0 \simeq 0.46$ eV [14] and $k_F^2 A/2\chi_Q^0 \simeq 0.4$ eV [12] we calculate that $B' \simeq 0.35$ eV$^{1/2}$ and $C \simeq 0.4$ eV. The fitted parameter values agree with the values that are calculated from the basic physical parameters of the model, i.e. the choice of the parameters is reasonable. Therefore the fit is satisfactory.

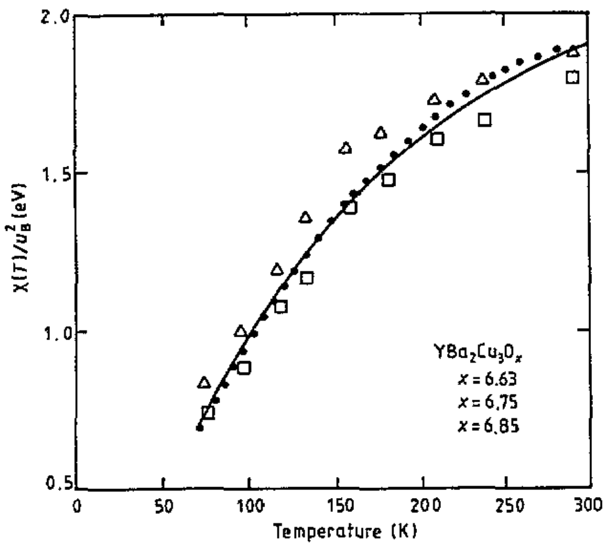

Figure 3. $\chi(T)$ versus T: ——, from equation (3.2); ●, experimental data from [19]; △, □, experimental data from [18].

For $La_{1.85}Sr_{0.15}CuO_4$ ($T_c = 38$ K) a least-squares fit of the theoretical equation (3.1) to the experiment [17, 20] yields the following result:

$$\chi(T) = 3.47 - \frac{20.15}{(T+75)^{1/2}} \tan^{-1}\left(\frac{70}{(T+75)^{1/2}}\right). \tag{3.3}$$

In figure 4 a plot of $\chi(T)$ versus T for $La_{1.85}Sr_{0.15}CuO_4$ is shown. The solid curve shows the values from equation (3.3). The following values are used for the parameters in the fit: $\chi^0 = 3.47$ eV^{-1}, $B' = 0.15$ eV$^{1/2}$ and $C = 0.272$ eV. On the other hand by using $I^2 N_0 \simeq 0.22$ eV [14] and $k_F^2 A/2\chi_Q^0 \simeq 0.3$ eV [12] we calculated that $B' \simeq 0.22$ eV$^{1/2}$ and $C \simeq 0.3$ eV. The fitted parameter values agree with the values that are calculated from the basic physical parameters of the model, i.e. the choice of the parameters is reasonable. Therefore the fit is also satisfactory.

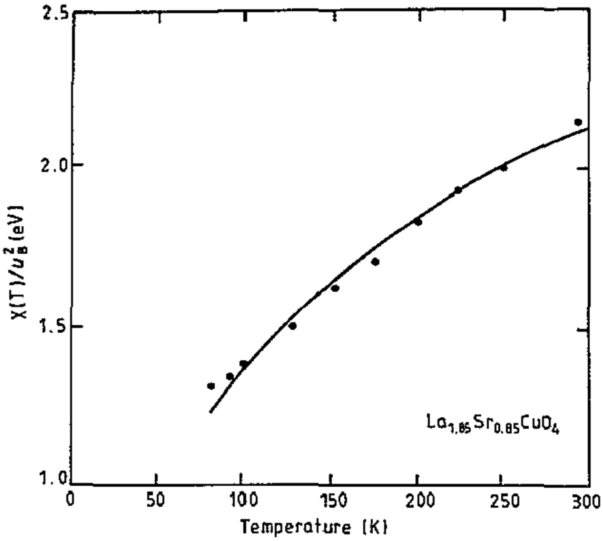

Figure 4. $\chi(T)$ versus T: ——, from equation (3.3); ●, experimental data from [20].

For the overdoped region ($YBa_2Cu_3O_7$) its uniform spin susceptibility is nearly temperature independent. This can be explained by assuming that the averaging of $\mathrm{Re}[\Sigma_1(p_F, \omega)]$ over its Fermi surface is nearly temperature independent, i.e.

$$\mathrm{Re}\left[\overline{\Sigma_1(p_F, \omega)}\right] = -3\omega\lambda'$$

with

$$\lambda' \sim I^2 N_0 \frac{\chi_Q^0}{\sqrt{2}\pi A|k_F|^2} \tan^{-1}\left(\frac{|k_F|^2}{2}\right)^{1/2}.$$

Thus we have

$$\chi(T) = \chi^0 - \chi^0 I^2 N_0 \frac{\chi_Q^0}{\sqrt{2}\pi A|k_F|^2} \tan^{-1}\left(\frac{|k_F|^2}{2}\right)^{1/2}. \tag{3.4}$$

This is nearly temperature independent. Using $I^2N_0 = 0.8$ eV [21], $|k_F|^2 = 4\pi$ and $|k_F|^2 A/2\chi_Q^0 = 0.8$ eV [12] and $\chi^0 = 3\ \mathrm{eV}^{-1}$ from equation (3.4), we get $\chi(T) = 2.6\ \mathrm{eV}^{-1}$ which also agrees with the experimental value of 2.62 eV [18].

4. Summary

In this paper we developed a theory of the effect of antiferromagnetic spin fluctuations on the uniform spin susceptibility and found a formula which reflects the effect of antiferromagnetic spin fluctuations on the uniform spin susceptibility. Our theoretical analysis fits the experimental results excellently and suggests strongly that the effect of the antiferromagnetic spin fluctuations on the uniform spin susceptibility is the origin of the temperature dependence of uniform spin susceptibility in high-T_c superconductors.

Acknowledgment

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